Pecazine M (nor-), monoacetylated

Inchi: InChI=1S/C20H22N2OS/c1-15(23)21-12-6-7-16(13-21)14-22-17-8-2-4-10-19(17)24-20-1
InchiKey: ROZGHCNCKBTUAX-UHFFFAOYSA-N
Formula: C20H22N2OS
SMILES: CC(=O)N1CCCC(CN2c3ccccc3Sc3ccccc32)C1
Mol. weight [g/mol]: 338.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	4.548		Crippen Method
mcvol	261.300	ml/mol	McGowan Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310442&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.